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AUTHOR(S):

Murota, Kazuo

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IMT-type Quadrature Formulas Free from Intrinsic Errors

定数関数に対し正確な値を与えるIMT型数値積分公式

Kazuo Murota

Institute of Socio-Economic Planning, University of Tsukuba

筑波大 社会工学系 室田一雄

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Abstract Let $x=\psi(t)$ ($\psi(0)=0$, $\psi(t)+\psi(1-t)=1$) be an IMT-type transformation for the numerical integration of $\int_0^1 f(x)dx$. This note points out that the transformation $x=\tilde{\psi}(t)$, where $\tilde{\psi}(t) = \int_0^{2t} \psi(s)ds$ ($0 \leq t \leq 1/2$) and $\tilde{\psi}(t)+\tilde{\psi}(1-t)=1$, leads to a quadrature formula which is free from the intrinsic error (i.e., exact for $f(x)=1$) and as efficient as the original quadrature formula based on $x=\psi(t)$.

1. Introduction

We consider the numerical integration of

$$I = \int_0^1 f(x)dx. \quad (1.1)$$

A numerical quadrature formula based on the change of variable $x=\psi(t)$ ($\psi(a)=0$, $\psi(b)=1$, $\psi'(a)=\psi'(b)=0$) is obtained by applying the trapezoidal rule to the transformed integral

$$I = \int_a^b f(\psi(t))\psi'(t)dt. \quad (1.2)$$

Among such formulas, the IMT formula [Iri-Moriguti-Takasawa 1970] and the DE (Double Exponential) formula [Takahasi-Mori 1974] are well known (cf. [Davis-Rabinowitz 1984], [Mori 1985]). The former employs

$$\psi_{\text{IMT}}(t) = (1/Q) \int_0^t \exp[-1/s - 1/(1-s)] ds, \quad (1.3)$$

$$Q = \int_0^1 \exp[-1/s - 1/(1-s)] ds$$

as the function $\psi(t)$ to map the interval $(0,1)$ onto itself (i.e., $a=0$, $b=1$ in (1.2)), and the latter adopts

$$\psi_{\text{DE}}(t) = (1/2) \tanh[(\pi/2) \sinh t] + 1/2, \quad (1.4)$$

which maps $(a,b)=(-\infty, \infty)$ onto $(0,1)$.

The resulting quadrature formula in the case of $(a,b)=(0,1)$ is then given by

$$S_N = h \sum_{i=1}^{N-1} f(\psi(ih)) \psi'(ih), \quad (1.5)$$

where $h=1/N$. In the case of $(a,b)=(-\infty, \infty)$, on the other hand, the trapezoidal approximation to (1.2) (with mesh size h)

$$S = h \sum_{i=-\infty}^{\infty} f(\psi(ih)) \psi'(ih) \quad (1.6)$$

involves infinitely many points (abscissas), which should be truncated to a finite number, say N , without deteriorating the degree of approximation; S_N will denote a sum of the form (1.6) with N terms.

We will define

$$E_N = E_N(f) = S_N - I, \quad (1.7)$$

which is the integration error for an integrand $f(x)$. It is known that the IMT formula and the DE formula have the property:

$$E_N \text{ decreases faster than any polynomial in } 1/N \text{ as } N \rightarrow \infty \text{ for a class of integrands of practical interest that may possess integrable algebraic/logarithmic singularities at endpoints of interval of integration.} \quad (1.8)$$

One of the peculiar properties of such a quadrature formula is that it fails to integrate a constant function exactly, that is,

$$E_N(1) \neq 0. \quad (1.9)$$

The error $E_N(1)$ is called the intrinsic error of the formula, which we are particularly concerned with here. Both the IMT formula and the DE formula, as well as their variants [Mori 1978], [Murota-Iri 1982], do have the property (1.9). In fact, all the formulas based on the technique of change of variable found in the literature (cf., e.g., [Takahasi-Mori 1973], [Mori 1985]) have this property, too.

Very recently, however, it was pointed out by Prof. Iri (reported in [Nishii-Murota-Iri 1985]) that there exists such a transformation function $\psi(t)=\psi_U(t)$ that yields a quadrature formula which has the property (1.8) and is free from intrinsic errors, i.e.,

$$E_N(1) = 0 \quad \text{for } N \text{ even.} \quad (1.10)$$

The function $\psi_U(t)$ is the cumulative distribution function of the random variable

$$\sum_{j=1}^{\infty} U_j / 2^j \quad (1.11)$$

where U_j ($j=1,2,\dots$) are independent random variables each being subject to the uniform distribution over the unit interval $(0,1)$. It can be shown [Iri-Kabaya 1985] that $\psi_U(t)$ satisfies the functional equation

$$\psi_U(t) = \int_0^{2t} \psi_U(s) ds \quad (0 \leq t \leq 1/2), \quad (1.12)$$

$$\psi_U(t) + \psi_U(1-t) = 1.$$

See [Iri-Kabaya 1985] for other properties of $\psi_U(t)$.

Unfortunately, the quadrature formula using $\psi_U(t)$ turned out [Nishii-Murota-Iri 1985] to be far less efficient for general integrands $f(x)$ than the IMT-type formulas, as compared in Table 1.1. This note gives quadrature formulas with no intrinsic errors that are roughly as efficient as the known IMT-type formulas.

Table 1.1. Efficiency and Intrinsic Errors

(a,b)	Formula	Efficiency (Error $E_N(f)$)	Intrinsic Error $E_N(1)$
finite	$\psi_U(t)$	$\exp[-c(\log N)^2]$	0
(0,1)	IMT: $\psi_{\text{IMT}}(t)$	$\exp[-c\sqrt{N}]$	same as $E_N(f)$
	IMT-type DE*	$\exp[-cN/(\log N)^2]$	same as $E_N(f)$
	IMT-double**	$\exp[-cN/(\log N)^2]$	same as $E_N(f)$
	IMT-triple**	$\exp[-cN/(\log N (\log \log N)^2)]$	same as $E_N(f)$
infinite ($-\infty, \infty$)	DE: $\psi_{\text{DE}}(t)$	$\exp[-cN/(\log N)]$	same as $E_N(f)$

* [Mori 1978]; ** [Murota-Iri 1982]

2. Intrinsic-Error Free Formulas

In the following, we assume

$$\begin{aligned} \psi(0)=0, \psi(1)=1 \quad (\psi(t)=0 \text{ for } t<0, \psi(t)=1 \text{ for } t>1), \\ \psi(t) + \psi(1-t) = 1, \end{aligned} \quad (2.1)$$

$$\psi'(0)=\psi'(1)=0 \quad (\psi(t) \text{ is differentiable as many times as needed}).$$

The Fourier transform of $\psi'(t)$ is defined by

$$\omega(\kappa) = \int_0^1 \psi'(t) \exp(i2\pi\kappa t) dt, \quad \kappa \in \mathbb{R}. \quad (2.2)$$

The error $E_N(f)$ is expressed (see, e.g., [Murota-Iri 1982]) in terms of the Fourier coefficients $C_k = C_k(f)$ of the integrand of (1.2):

$$E_N(f) = 2 \sum_{p=1}^{\infty} \operatorname{Re} C_{pN}(f), \quad (2.3)$$

$$C_k(f) = \int_0^1 f(\psi(t))\psi'(t)\exp(i2\pi kt)dt, \quad k \in \mathbb{Z}. \quad (2.4)$$

The intrinsic error is then given by

$$E_N(1) = 2 \sum_{p=1}^{\infty} \omega(pN). \quad (2.5)$$

This expression indicates that if

$$\omega(2k) = 0 \quad (k=1,2,\dots), \quad (2.6)$$

then the formula with $x=\psi(t)$ has no intrinsic errors for N even.

It is a rule of thumb that the efficiency for a general integrand $f(x)$ is measured by how fast $|\omega(\kappa)|$ decays as $|\kappa| \rightarrow \infty$. In fact, this is the case with the IMT-type formulas. We discuss this issue in Appendix.

Now our problem of designing an efficient intrinsic-error free quadrature formula is reduced to that of finding such a Fourier transform $\omega(\kappa)$ of a nonnegative function $\psi'(t)$ (or, a characteristic function of a symmetric probability distribution) that satisfies (2.6) and decreases as rapidly as possible as $|\kappa| \rightarrow \infty$.

Here we take notice of the following facts:

(1) The Fourier transform of $\psi'_U(t)$ (or, the characteristic function of (1.11)) is given by

$$\omega_U(\kappa) = \exp(i\pi\kappa) \prod_{j=1}^{\infty} \sin(\pi\kappa/2^j)/(\pi\kappa/2^j), \quad (2.7)$$

which satisfies (2.6) on account of the factor $\sin(\pi\kappa/2)/(\pi\kappa/2)$. That is, the factor corresponding to $U_1/2$ in (1.11) renders the quadrature formula using $\psi_U(t)$ free from intrinsic errors.

(2) The Fourier transform $\omega(\kappa)$ of the derivative of an IMT-type transformation function $\psi(t)$ tends to zero rapidly as $|\kappa| \rightarrow \infty$; e.g., for (1.3), it is known [Iri-Moriguti-Takasawa 1970] that

$$\omega_{\text{IMT}}(\kappa) = O(\exp[-c\sqrt{|\kappa|}]). \quad (2.8)$$

(3) The product of two characteristic functions is again a characteristic function of a probability distribution.

When given an efficient quadrature formula based on a transformation $x=\psi(t)$, we can construct an intrinsic-error free formula using the transformation $x=\tilde{\psi}(t)$ defined as follows. Let $\omega(\kappa)$ and $\tilde{\omega}(\kappa)$ be the Fourier transforms of $\psi'(t)$ and $\tilde{\psi}'(t)$, respectively. We define

$$\tilde{\omega}(\kappa) = \omega(\kappa/2) \exp(i\pi\kappa/2) \sin(\pi\kappa/2) / (\pi\kappa/2) \quad (2.9)$$

and $\tilde{\psi}'(t)$ to be the inverse Fourier transform of $\tilde{\omega}(\kappa)$. In terms of $\psi(t)$ and $\tilde{\psi}(t)$, this amounts to

$$\tilde{\psi}(t) = \int_0^{2t} \psi(s) ds \quad (0 \leq t \leq 1/2), \quad (2.10)$$

and

$$\tilde{\psi}(t) + \tilde{\psi}(1-t) = 1. \quad (2.11)$$

Then it is easy to see, based on the above-mentioned facts, that $x=\tilde{\psi}(t)$ is qualified as the transformation function satisfying (2.1), and that the resulting quadrature formula is free from intrinsic errors and roughly as efficient as the original formula with $x=\psi(t)$. To be more precise, the new formula will require at most twice as many function evaluations as the original one, since we have

$$|\tilde{\omega}(\kappa)| \leq |(2/\pi\kappa) \omega(\kappa/2)|, \quad \kappa \neq 0, \quad (2.12)$$

from (2.9). Namely, we may expect the relation

$$|\tilde{E}_N(f)| \leq |E_{N/2}(f)| \quad (2.13)$$

between the integration error \tilde{E}_N of the new formula and that of the original one.

When $\psi(t)$ is a polynomial, the explicit form of $\tilde{\psi}(t)$ can be given; for example, when

$$\psi'(t) = ((2m+1)!/(m!)^2) t^m(1-t)^m, \quad m=2,3,$$

we have

$$\tilde{\psi}(t) = 8t^4(5-12t+8t^2) \quad (0 \leq t \leq 1/2) \quad \text{for } m=2,$$

and

$$\tilde{\psi}(t) = 32t^5(7-28t+40t^2-20t^3) \quad (0 \leq t \leq 1/2) \quad \text{for } m=3.$$

It may worth while noting that (1.12) shows that $\psi_U(t)$ is a fixed point of the transformation (2.10), i.e.,

$$\tilde{\psi}_U(t) = \psi_U(t).$$

3. Numerical Examples

We compare the quadrature formulas with $x=\psi(t)$ and $x=\tilde{\psi}(t)$ (cf.

(2.10)) for the two choices $\psi(t) = \psi_{\text{TANH}}(t)$ and $\psi(t) = \psi_{\text{IMTDE}}(t)$, where

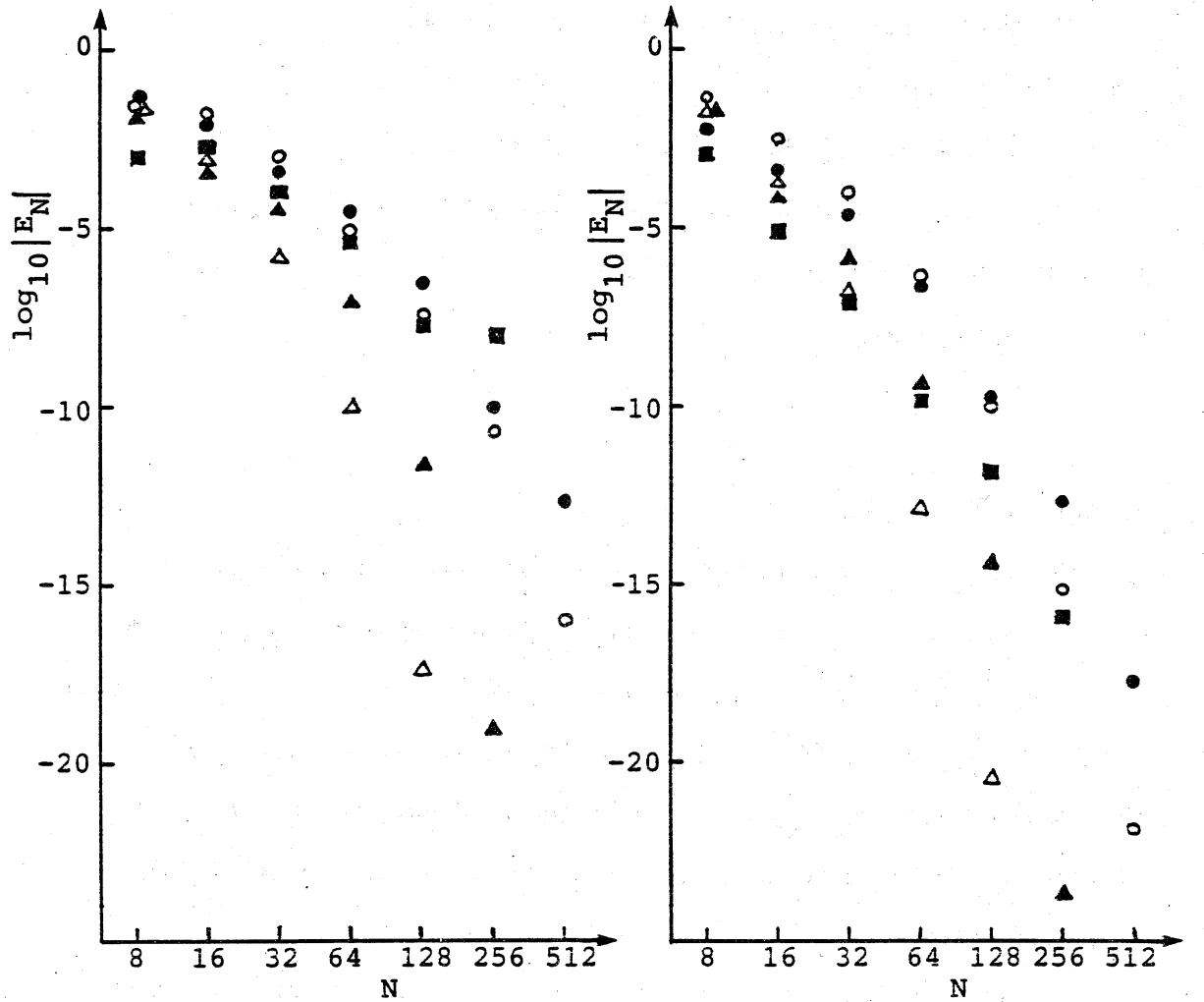
$$\psi_{\text{TANH}}(t) = (1/2)\tanh[(1/4)(1/(1-t)-1/t)] + 1/2, \quad (3.1)$$

$$\psi_{\text{IMTDE}}(t) = (1/2)\tanh[(\pi/2)\sinh[(\pi/4)(1/(1-t)-1/t)]] + 1/2. \quad (3.2)$$

The formula with $x=\psi_{\text{IMTDE}}(t)$ is the IMT-type double exponential formula of [Mori 1978]. The formula with $x=\psi_U(t)$ [Nishii-Murota-Iri 1985] is also considered.

The integration errors are observed for the following six integrand functions:

$f_1(x) = 1,$	$I = 1,$
$f_2(x) = \exp x,$	$I = e-1 = 1.7182\dots,$
$f_3(x) = x^2,$	$I = 1/3 = 0.3333\dots,$
$f_4(x) = 1/\sqrt{x},$	$I = 2,$
$f_5(x) = (\log x)/(x^2-1.5x+1.25),$	$I = -1.0518\dots$
$f_6(x) = 2/(1+(2x-1)^2),$	$I = \pi/2 = 1.5707\dots$



(1) Errors for $f_4(x) = 1/\sqrt{x}$

(2) Errors for $f_5(x) = \frac{\log x}{x^2 - 1.5x + 1.25}$

Fig. 3.1. Numerical integration based on the transformation $x=\psi(t)$

$\circ : \psi_{\text{TANH}}(t)$ $\bullet : \tilde{\psi}_{\text{TANH}}(t)$
 $\triangle : \psi_{\text{IMTDE}}(t)$ $\blacktriangle : \tilde{\psi}_{\text{IMTDE}}(t)$
 $\blacksquare : \psi_U(t)$

The computations are done with mantissa of 28 hexadecimal digits by HITAC M-170H.

Fig. 3.1 illustrates the integration errors for $f_4(x)$ and $f_5(x)$ against the number of function evaluations. Similar results are obtained for other integrands. Note that (2.13) is verified.

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Appendix

We discuss the validity of the claim that

if $|\omega(\kappa)|$ decreases fast as $|\kappa| \rightarrow \infty$, then so does $|E_N(f)|$
as $N \rightarrow \infty$ for a well-behaved integrand $f(x)$.

The following proposition, combined with (2.3), implies that the above claim holds true for polynomial integrands $f(x)=x^m$ in the particular case of $\psi(t)=\psi_{\text{IMT}}(t)$ (cf. (2.8)). Note that the proof is such that it can be adapted to other transformation functions $\psi(t)$ once bounds on $|\omega(\kappa)|$ and $|\omega'(\kappa)|$ are obtained.

Proposition A.1. Let $\psi(t)$ satisfy (2.1) and put

$$C_k = \int_0^1 \psi'(t) \exp(i2\pi kt) dt, \quad k \in \mathbb{Z}, \quad (\text{A.1})$$

$$D_k = \int_0^1 t \psi'(t) \exp(i2\pi kt) dt, \quad k \in \mathbb{Z}, \quad (\text{A.2})$$

$$C_k^m = \int_0^1 \psi(t)^m \psi'(t) \exp(i2\pi kt) dt, \quad k \in \mathbb{Z}, m \in \mathbb{Z}_+. \quad (\text{A.3})$$

If

$$|C_k| \leq A \exp(-B \sqrt{|k|}), \quad k \in \mathbb{Z}, \quad (\text{A.4})$$

$$|D_k| \leq A \exp(-B \sqrt{|k|}), \quad k \in \mathbb{Z}, \quad (\text{A.5})$$

where A and B are constants independent of k, then

$$|C_k^m| \leq A_m |k| \exp(-B \sqrt{|k|}), \quad k \in \mathbb{Z} \setminus \{0\}, \quad (\text{A.6})$$

where A_m is defined by

$$A_0 = A; \quad A_{m+1} = A[3/2 + (m+1)(1+4/B^2)A_m/(2\pi)], \quad m=0,1,\dots \quad (\text{A.7})$$

Proof: Firstly, put

$$a_k^m = \int_0^1 (\psi(t)^m - t) \exp(i2\pi kt) dt, \quad k \in \mathbb{Z}, \quad m \in \mathbb{Z}_+. \quad (\text{A.8})$$

We have

$$a_0^1 = 0 \quad (\text{A.9})$$

and

$$-1/2 \leq a_0^m \leq 0, \quad (\text{A.10})$$

since

$$a_0^m = \int_0^1 (\psi(t)^m - t) dt = \int_0^1 \psi(t)^m dt - 1/2$$

and

$$0 \leq \int_0^1 \psi(t)^m dt \leq \int_0^1 \psi(t) dt = 1/2.$$

For $k \in \mathbb{Z} \setminus \{0\}$, integration by parts yields

$$\begin{aligned} a_k^m &= [(\psi(t)^m - t) \exp(i2\pi kt) / (i2\pi k)]_{t=0}^1 \\ &\quad - \int_0^1 (m\psi(t)^{m-1} \psi'(t) - 1) \exp(i2\pi kt) / (i2\pi k) dt \\ &= -(m/i2\pi k) \int_0^1 \psi(t)^{m-1} \psi'(t) \exp(i2\pi kt) dt \\ &= -(m/i2\pi k) C_k^{m-1}. \end{aligned} \quad (\text{A.11})$$

Now we will establish (A.6) by induction with respect to m using the following identity:

$$C_k^{m+1} = D_k + a_0^{m+1} C_k - ((m+1)/i2\pi) \sum_{j \neq 0} C_j^m C_{k-j} / j, \quad (\text{A.12})$$

which follows from

$$\begin{aligned} C_k^{m+1} &= \int_0^1 (\psi(t)^{m+1} - t) \psi'(t) \exp(i2\pi kt) dt + \int_0^1 t \psi'(t) \exp(i2\pi kt) dt \\ &= \sum_{j=-\infty}^{\infty} a_j^{m+1} C_{k-j} + D_k \end{aligned}$$

combined with (A.11).

Basis (m=0): (A.6) for m=0 is obvious from (A.1), since $C_k^0 = C_k$ and $A_0 = A$.

Induction: Suppose (A.6) holds true for m. From (A.12) follows

$$|C_k^{m+1}| \leq |D_k| + |a_0^{m+1} C_k| + ((m+1)/2\pi) \sum_{j \neq 0} |C_j^m C_{k-j}/j|. \quad (A.13)$$

We have

$$|a_0^{m+1} C_k| \leq (A/2) \exp(-B \sqrt{|k|}) \quad (A.14)$$

from (A.4) and (A.10). The last part of (A.13) is estimated as follows by (A.4) and (A.6):

$$\begin{aligned} & \sum_{j \neq 0} |C_j^m C_{k-j}/j| \\ & \leq \sum_{j \neq 0} A_m |j| \exp(-B \sqrt{|j|}) \cdot A \exp(-B \sqrt{|k-j|}) / |j| \\ & = A_m A \sum_{j \neq 0} \exp[-B(\sqrt{|j|} + \sqrt{|k-j|})] \\ & = A_m A \left(\sum_{j=1}^{|k|} \exp[-B(\sqrt{j} + \sqrt{|k-j|})] + 2 \sum_{j=1}^{\infty} \exp[-B(\sqrt{j} + \sqrt{|k|+j})] \right) \\ & \leq A_m A (|k| + 4/B^2) \exp(-B \sqrt{|k|}), \end{aligned} \quad (A.15)$$

since

$$\sum_{j=1}^{|k|} \exp[-B(\sqrt{j} + \sqrt{|k-j|})] \leq \sum_{j=1}^{|k|} \exp(-B \sqrt{|k|}) = |k| \exp(-B \sqrt{|k|})$$

and

$$\begin{aligned} & \sum_{j=1}^{\infty} \exp[-B(\sqrt{j} + \sqrt{|k|+j})] \\ & \leq \exp(-B \sqrt{|k|}) \sum_{j=1}^{\infty} \exp(-B \sqrt{j}) \\ & \leq \exp(-B \sqrt{|k|}) \int_0^{\infty} \exp(-B \sqrt{x}) dx = 2 \exp(-B \sqrt{|k|}) / B^2. \end{aligned}$$

Substituting (A.5), (A.14) and (A.15) into (A.13), we obtain

$$|C_k^{m+1}| \leq A_{m+1} |k| \exp(-B \sqrt{|k|})$$

with A_{m+1} given by (A.7).

Q.E.D.

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